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Computer Modelling of Cyclic Deformation of High-Temperature Materials

TECHNICAL PROGRESS REPORT

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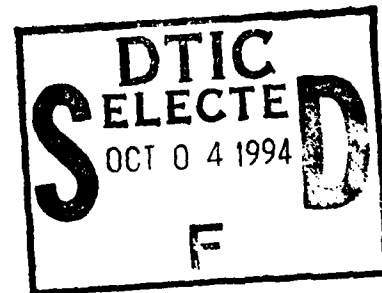
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I. Introduction and Program Objective

Current methods of lifetime assessment leave much to be desired. Typically, the expected life of a full-scale component exposed to a complex environment is based upon empirical interpretations of measurements performed on microscopic samples in controlled laboratory conditions. Extrapolation to the service component is accomplished by scaling laws which, if used at all, are empirical; little or no attention is paid to synergistic interactions between the different components of the real environment. With the increasingly hostile conditions which must be faced in modern aerospace applications, improvement in lifetime estimation is mandated by both cost and safety considerations.

This program aims at improving current methods of lifetime assessment by building in the characteristics of the micro-mechanisms known to be responsible for damage and failure. The broad approach entails the integration and, where necessary, augmentation of the micro-scale research results currently available in the literature into a macro-scale model with predictive capability.

In more detail, the program will develop a set of hierarchically structured models at different length scales, from atomic to macroscopic, at each level taking as parametric input the results of the model at the next smaller scale. In this way the known microscopic properties can be transported by systematic procedures to the unknown macro-scale region. It may not be possible to eliminate empiricism completely, because some of the quantities involved cannot yet be estimated to the required degree of precision. In this case the aim will be at least to eliminate functional empiricism. Restriction of empiricism to the choice of parameters to be input to known functional forms permits some confidence in extrapolation procedures and has the advantage that the models can readily be updated as better estimates of the parameters become available.

II. Program Organization

The program has been organized into specific tasks and subtasks as follows.

Task 100. Lifetimes of metallic dispersed-phase composites

Most service materials fall into the category of dispersion-hardened metallic composites. This task will consider the problem of dispersion hardened materials in general, but with two specific materials, NiAl and MoSi₂/SiC in mind.

Task 110. Identification and modelling of micromechanisms

The purpose of this task is to determine what micromechanisms are operative in the high-temperature deformation of dispersion-hardened materials. In the general case this will be done by a literature search. For specific materials, the micromechanisms will be determined from the experimental program at NRL. Once identified, each of these micromechanisms will be modelled, in order to determine what are the critical parameters which determine its effect on plastic flow and values for these parameters. Also to be determined is whether the modelled critical values are dependent on

quantities which must be obtained from a smaller scale model.

Task 111. Equiaxed dispersoids

This task will consider dispersions of the type encountered in NiAl-like materials. That is, the dispersoids are considered to be small compared to the grain size. The term 'equiaxed' is used because the particles are roughly of the same size in all three dimensions. However, this is not a requirement for this task. Rather, it is necessary that the particles not be too large in the dimension normal to the slip plane, so that they can be surmounted with relative ease by cross-slip and/or climb without the generation of appreciable back-stress.

Task 112. Anisotropic dispersoids

This task covers the case of dispersoids which are elongated in the direction normal to the slip plane. An example is SiC fibers in MoSi₂. In this case, plastic flow around the dispersoids takes place by a combination of glide and climb, but is a protracted process during which large stresses acting in opposition to the applied load are developed.

Task 113. Grain boundary effects

This task will examine the role of grain boundary processes in high-temperature deformation.

Task 120. Macroscopic stochastic model for creep

In real materials it is likely that more than one mechanism will be operative, either in parallel or in series. The information gained in task 110 is not sufficient to describe this situation. Once the critical parameters for individual mechanisms have been determined, it is necessary to combine them in a macroscale stochastic model. This will be done by determining critical stresses and activation enthalpies as a function of local geometry and using these values in a finite-temperature simulation of creep through a random array of dispersoids. Careful attention must be paid to possible interactions between mechanisms.

Task 130. Extension to cyclic deformation

The final step in task 100 is to extend the results to the case of cyclic deformation. Irreversibility is an intrinsic feature of the model in task 120. However, it is likely that other, as yet unrecognized, characteristics of cycled deformation will have to be considered.

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Task 200. Lifetimes of piezoelectric ferroelectrics

Failure in cyclic loading of sensors and actuators formed from lead zirconate titanate (PZT) is a continuing problem. PZT is a ceramic and therefore differs from the materials considered in task 100 in that plastic deformation is not involved. This task will examine, modelling as necessary, the operation of PZT devices, in order to determine the factors governing lifetime limitation.

Task 300. Reporting

Running concurrently with tasks 100 and 200, this task will inform the Navy Program Manager and Contracting Officer of the technical and fiscal status of the program through R&D status reports.

III. Technical Progress

Task 112. Anisotropic dispersoids

Experiment shows that creep for dispersed-phase alloys is thermally activated and that the strain rate is very strongly dependent on stress. This latter feature is particularly marked at small stresses. This observation and the utility of the idea has led to the introduction of the notion of a threshold stress. Thus, it is envisaged that the strain rate below some critical stress is zero. Unfortunately this postulate and the existence of thermal activation are incompatible. Here we shall accept that thermal activation is of dominant importance and shall accordingly reject the existence of a critical stress.

We now proceed to develop a model of creep which accords with this basic premise. We observe first that at elevated temperatures and for the case of an applied tension all dislocations, both edge and screw, (down) climb uniformly under the action of the local normal stress. In general this stress is such that the rate of climb is vanishingly small. However, this is not the case when the motion of a gliding dislocation is halted locally by the presence of impenetrable particles. In the simplest case, that is, when the particle has the same modulus as the matrix and fits without distortion into the hole which it occupies in the lattice, the gliding dislocation will, over a short length, bend into a circular arc having the radius of curvature defined by the radius, r_c , of the circle of intersection of the glide plane of the dislocation with the particle. The stress acting over the curved length is

$$\tau + \frac{\mu}{r_c}$$

over r_c where τ is the applied shear stress, μ is the shear modulus and b is the magnitude of the Burgers vector. The associated force is

$$\tau r_c \sin \theta = \sigma \lambda$$

where 2θ is the angle subtended at the centre of the circle of intersection by the arc at the surface of the particle and λ is the separation of adjoining particles. The force for climb over this length is easily shown to be

$$\sigma \lambda [1 + \cos \phi + \sin \phi] \quad (1)$$

where ϕ is the angle between the tangent at the line of contact and the glide plane. We now suppose, since the rate of climb is generally small, that dislocations are confined to the original glide plane over most of the length between obstacles. We further suppose that within the lengths $2r_c \sin \theta$ they conform roughly to the shape of the obstacles. Thus, one expects that, in these regions, dislocations are curved in both horizontal and vertical planes. The complications consequent on this feature are such that it is necessary in the first instance to resort to approximations in the model. To do this and retain acceptable accuracy one must first identify the essential physics of the situation. These appear to be: dislocation climb is localized in the neighborhood of the particles; the force for climb derives

mainly from the force for glide on the whole dislocation length λ and; the path chosen is that of least resistance.

Thus, we ignore the curvature in the horizontal plane. Further, we suppose that the climbing dislocation forms an arc of a circle of radius R which contacts the obstacle at a height h above the glide plane and that the climb force is applied uniformly over its length. This force is that given by (1) less that due to the fact that the dislocation is bent. Taking the projected length as l we have:

$$\sigma_c l = \tau \lambda (1 + \cos \phi + \sin \phi) - \frac{\mu b^2}{R}$$

Expressing l in terms of h and R this becomes:

$$\sigma_c = \frac{\tau \lambda (\cos \phi + \sin \phi + 1)}{\sqrt{2Rh - h^2}} - \frac{\mu b^2}{R\sqrt{2Rh - h^2}} \quad (2)$$

On the basis that $R \gg h$ the maximum is easily shown to occur when

$$R = \frac{2\mu b h}{\mu b - \tau \lambda (1 + \cos \phi + \sin \phi)}$$

Substituting for R in (2) we have a rather complicated expression for σ_c . For reasons which will become clear this is not expressed here.

Given a value for σ_c we are in principle in a position to determine the rate of climb and in particular the time to surmount a particle. Thus, we can express the rate of climb as

$$\dot{h} = \nu a e^{\frac{-U}{kT}} e^{\frac{\sigma_c \Omega}{kT}} \quad (3)$$

Here ν is the frequency of atomic vibrations, U is the energy for the formation and movement of a lattice vacancy, a is the atomic spacing between glide planes, Ω is the atomic volume, k is Boltzmann's constant and T is the absolute temperature. At this stage we have an expression which represents

$$\frac{dh}{dt} = f(h)$$

where $f(h)$ is the expression found on substituting for σ_c in (3).

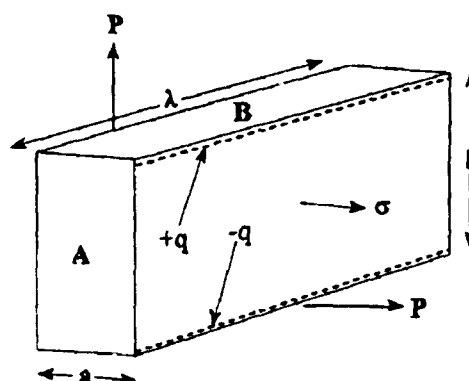
Inverting this equation and integrating with regard to h over the range of the particle radius results in the determination of the time to surmount. Clearly, such an evaluation is beyond the scope of algebraic manipulation and the evaluation rests on the use of numerical integration. This is work which will be next addressed.

Task 200. Lifetimes of piezoelectric ferroelectrics

Mobility of 90° Domain Walls

The mobility of 90° domain walls (assumed to lie on {100} planes) in the limit of pinning by dislocations has been treated in an earlier report. In the last report the treatment of unpinned walls was begun. The unpinned walls are not restricted to lie on {100} planes, but can equally well arise as boundaries between domains with a twin relationship. In this report this treatment will be continued; for convenience and continuity, part of the initial discussion contained in the last report will be repeated here.

A 90° domain wall is the interface between tetragonal crystal lattices oriented with c-axes at right angles to each other. An electric field is directed parallel to the c-axis and thus the direction but not the intensity of the electric field changes at a 90° domain wall. Movement of a wall in a direction normal to itself then necessarily requires a change in both lateral dimensions and in the direction of the local electric field in the volume swept as a consequence of the motion. The domain wall configuration (and hence its energy also) are invariant to translation through an integral number of lattice spacings. That is, the energy is



periodic with the period of the lattice. In the absence of an atomistic calculation it is not possible to estimate the energy of a domain wall at a position lying between its periodic minima, but the experimental observation that the walls are straight suggests that this energy is relatively large. Therefore it seems likely that the situation is analogous to that of dislocation mobility in most crystalline solids - that the mechanism of mobility is the formation of a nucleus and its subsequent growth. In the case of dislocations, the nucleus is an advance of a small length of the line through a single atomic spacing, forming an excitation known as a kink pair. By analogy, the nucleus for a domain wall is a "pillbox"-like small area of the wall advanced through a unit step into an adjacent domain. This is illustrated in Figure 1, in which an area of dimensions $\lambda \times h$ has been moved through a distance a from left to right (in the diagram) from a domain in which the polarization P is vertical into one in which the polarization is horizontal. A normal stress σ is considered to act on the wall. Because the normal component of the electric displacement must be continuous across the faces B,

layers of depolarization charge density $\pm q$ (dashed lines in Figure 1) of uncertain magnitude develop on these interfaces. The enthalpy of the "pillbox" can be written in the form

$$H = 2aE_w(2h+\lambda) + E_{es} - 2\sigma h\lambda a\eta \quad (4)$$

where the first term is the energy of the sidewalls A and B of the pillbox (E_w is the wall energy per unit area and it is assumed that the walls B and A are of type I and II, respectively) and E_{es} is the electrostatic energy. The third term is the work done by the wall stress in forming the pillbox (η is the misfit parameter). The wall energy E_w can be expressed in terms of η by supposing that a single layer of material at the domain wall is strained elastically to a cubic shape, so that

$$E_w = \mu a\eta^2 \quad (5)$$

where μ is the shear modulus. The value of E_w predicted by (5) varies from 2.5 to 10 mJ m⁻² as η rises from 0.02 to 0.04, and is in good agreement with previous estimates of 5 to 7 mJ m⁻².

The electrostatic energy consists of three terms. First, the energy of the repolarized material within the pillbox, which is

$$E_I = \frac{1}{2} h\lambda a \frac{P^2}{\kappa\kappa_0} \quad (6)$$

where P is the remanent polarization per unit volume, κ is the dielectric constant and κ_0 is the permittivity of free space. P can also be expressed in terms of the misfit parameter η by normalizing to a value of 0.2 C m⁻² for 75% polarization at $\eta = 0.035$ (for Pb(Zr_{0.5}Ti_{0.5})O₃) from which there results

$$P = 7.62 \eta \quad (7)$$

Second, the self-energy of the depolarizing dipole layer, given by

$$E_{II} = \frac{q^2}{\kappa\kappa_0} \int_0^\lambda d\lambda_1 \int_0^\lambda \frac{d\lambda_2}{\sqrt{h^2 + (\lambda_2 - \lambda_1)^2}} \quad (8)$$

and finally, the interaction energy between the depolarizing dipole layer and the remanent polarization,

$$E_{III} = -\frac{qh\lambda P}{\kappa\kappa_0} \quad (9)$$

The only one of these terms which requires any effort in evaluation is E_{II} in (8), which can be

rewritten in parametric form

$$E_H = \frac{q^2}{\kappa\kappa_0} I$$

$$I = h \int_0^{\frac{\lambda}{h}} \int_{-\frac{\lambda}{h}}^{\frac{\lambda}{h}-s} \frac{dt}{\sqrt{(1+t^2)^2}}$$
(10)

in which the double integral $I/h(\lambda/h)$ can readily be evaluated numerically by gaussian quadrature. The functional form of this integral was shown in the last report and will not be repeated here.

The major uncertainty in the treatment above is the magnitude of the depolarization charge q . For present purposes it has been assumed that charges $\pm q$ across a unit cell will form a dipole of moment commensurate with that of the intrinsic dipole, p ; that is, that $q=p/a$. It is probable that this figure is correct to better than an order of magnitude. It is found that the contribution of the terms containing q to the total enthalpy is no more than 12%, so that the depolarization terms are of secondary importance.

A typical pillbox enthalpy surface is shown in Figure 2. The reduced enthalpy $H/\mu a^3$ is shown as a function of width λ and height h for a misfit of $\eta=0.010$ and an applied stress of 0.001μ . There is a saddle point, the activation enthalpy, with a magnitude of $9.7 \times 10^{-3} \mu a^3$ at $h=9a$ and $\lambda=5a$. For $\mu=150\text{GPa}$ and $a=0.4\text{nm}$, the value for the activation enthalpy is 0.058eV . This would permit a wall velocity of order 10^9a s^{-1} at 100K , compatible with the experimental observation that there is a piezoelectric response to a 1GHz driving field at 100K .

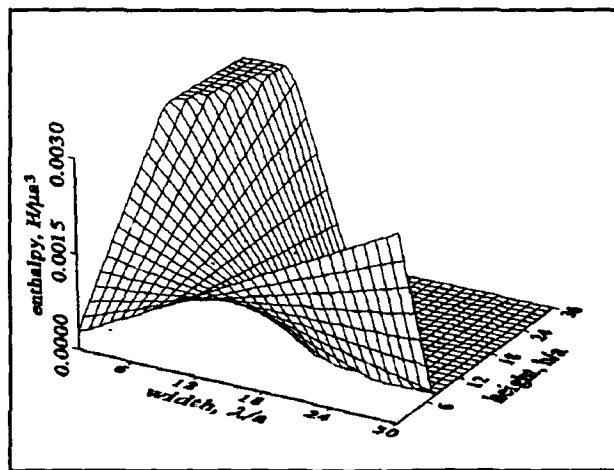


Figure 2 A typical pillbox enthalpy surface

No great significance, other than compatibility of the magnitudes, should be read into this agreement with experiment. The size of the activation enthalpy varies strongly with the applied stress and with the misfit parameter. This can be seen from Figure 3, in which the activation enthalpy is drawn as a function of misfit and applied stress, for misfit parameters from 0.010 to 0.025 and for applied stresses from $5 \times 10^{-4} \mu$ to $2 \times 10^{-3} \mu$. Clearly, while the activation energy can be small for low misfit and high stress, it can rise to as large a value as $0.025 \mu a^3$, or 0.15eV , for a misfit of 0.025 and an applied stress of $5 \times 10^{-4} \mu$.

In this state the piezoelectric response at 100K would die out for frequencies greater than 20kHz. The need to specify the misfit in experimental work is evident, yet very often this is not done. It is not sufficient to specify the Zr/Ti content, since the misfit changes from zero to 0.035 over a fraction of a percentage change in composition for PZT close to the morphotropic phase boundary.

It is worth noting that the kink mobility is not symmetric to tension and compression. Specifically, the interaction energy between the depolarizing dipole layer and the remanent polarization, E_m in (9), changes sign with the sense of deformation. This can be seen by reference to Figure 4. Two poled domains are drawn, each denoted by an arrow parallel to the poling direction; these are separated by an intermediate unpoled domain. Two kink pairs are shown. In the domain wall labelled A, the kink pair corresponds to motion of the wall *into* the poled domain, or to a horizontally applied tensile stress. The kink pair in the wall B is appropriate for movement of the wall *out of* the poled domain, and hence corresponds to a compression cycle. The "+" and "-" symbols indicate the signs of the depolarizing charge in both cases. It is clear that the interaction between the macroscopic polarization and the depolarization dipole will tend to contract the kink pair A, but to expand the kink pair B.

Therefore the effect of the depolarization asymmetry is to inhibit wall mobility in the tension cycle and to promote wall motion in the compression cycle. The magnitude of this asymmetry can be estimated by setting the enthalpy to be

$$H = H_0 \pm \Delta H \quad (11)$$

where ΔH is the asymmetric part (9). The differential velocity is then given by

$$\Delta v = v_- - v_+ = v_0 \left(1 - e^{\frac{-\Delta H}{kT}} \right) \quad (12)$$

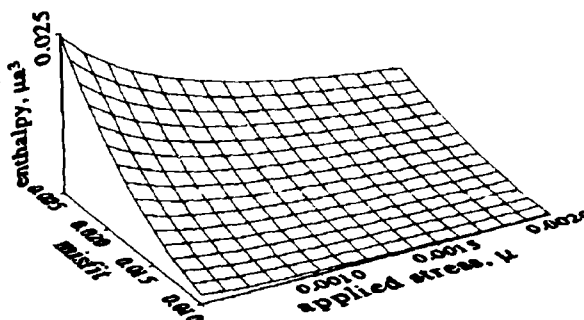


Figure 3 The activation enthalpy surface

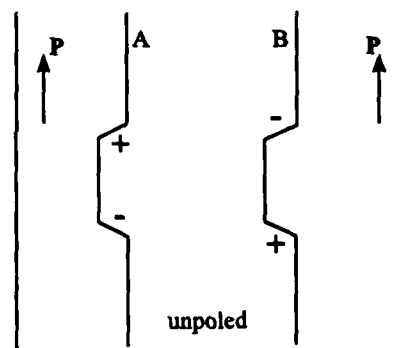


Figure 4 The asymmetry of kink pair mobility

The differential enthalpy surface is shown in Figure 5, for the same independent variables of misfit and stress as the absolute enthalpy in Figure 3. The differential term is typically 1-3% of the enthalpy, much too large to be responsible *by itself* for the observed lifetimes of cyclically deformed PZT. However, the magnitude of the differential enthalpy is directly proportional to q , the uncertainty of which has been emphasized above. Therefore it is considered a possibility that the asymmetry in the activation enthalpy for domain wall motion acts as a lifetime-limiting mechanism in cyclic deformation.

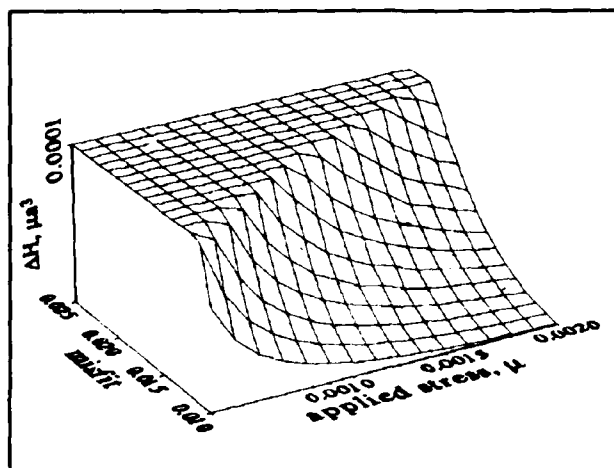


Figure 5 The differential activation enthalpy